# Molecular Docking Of 2-Azetidinones to Predict Therapeutic Potential

Ms. Yamini C Sonewane
*Gawande College of Pharmacy Sakharkherda, Tah Sindkhedraja, Dist. Buldhana*

***Abstract*—This study employs molecular docking simulations to assess the potential anti-ulcer and other therapeutic properties of novel 2-azetidinone derivatives, focusing on their binding affinities and interaction profiles with relevant target enzymes. This computational approach aims to identify lead compounds for further experimental validation by predicting their efficacy as inhibitors of established therapeutic targets, such as H+/K+-ATPase for anti-ulcer activity (Muhammad et al., 2019). This method enables the virtual screening of large libraries of compounds, providing insights into their molecular interactions with specific protein active sites (Azmatullah et al., 2022). Such in silico methods significantly accelerate the drug discovery process by prioritizing compounds with optimal binding characteristics, thereby reducing the time and cost associated with traditional experimental screening (Muhammad et al., 2019). The binding affinities are often quantified by docking scores (e.g., in kcal/mol), where a more negative score typically indicates a stronger interaction and thus a higher potential for therapeutic efficacy (Muhammad et al., 2019). For instance, compounds exhibiting binding energies around -9.1 kcal/mol against H+/K+-ATPase enzymes have demonstrated promising anti-ulcer activity (Muhammad et al., 2019). Furthermore, specific 2-azetidinone derivatives have shown significant binding energies, such as -9.4 kcal/mol with MMP-9 protein, suggesting potential anticancer activity through vigorous interactions including hydrogen bonds (Shweta et al., 2024). These interactions often involve key residues within the active site, forming stable protein-ligand complexes that can inhibit enzyme function. For example, specific monocyclic β-lactam ligands have demonstrated strong interactions with MMP-9, an enzyme associated with cancer proliferation, suggesting their potential as anticancer agents (Shweta et al., 2024). The visualization and analysis of these intermolecular interactions are crucial for understanding the binding strength and inhibitory potential, as proteins play a critical role in cellular functionality (Shweta et al., 2024). This predictive capability of molecular docking extends to various pathological conditions beyond cancer, including inflammatory and infectious diseases, by identifying compounds that can modulate the activity of crucial protein targets (Muhammad et al., 2019).**

***Index Terms*—chemical scaffold, computational methodology, and target-specific therapeutic areas.**

## I. INTRODUCTION

Molecular docking, a computational technique, plays a crucial role in predicting the binding affinity of small molecules to target proteins, thus offering insights into their potential therapeutic applications (Hassan et al., 2024). This method is particularly valuable for novel compounds such as 2-azetidinones, allowing for the in-silico evaluation of their interactions with target enzymes implicated in various pathologies like ulcers or cancer (Sulthana & Quine, 2015; Tripodi et al., 2018). By simulating the molecular recognition process, docking studies can identify optimal binding poses and estimate binding energies, which correlate with the strength of the ligand-protein interaction (Shweta et al., 2024). This predictive capability significantly accelerates the drug discovery pipeline by prioritizing promising candidates for further experimental validation, thereby reducing the time and cost associated with preclinical development (El-Saghier et al., 2023; Sulthana & Quine, 2015). The process typically involves constructing ligand structures using force fields like Optimized Potentials for Liquid Simulations-All Atom to compute partial atomic charges, followed by docking calculations performed with high precision modes, such as the "Extra Precision" setting in GLIDE (Sulthana & Quine, 2015). Furthermore, the comprehensive analysis of molecular docking results often involves visualizing molecular electrostatic potentials to

discern electrophilic and nucleophilic regions, which are critical for understanding ligand-protein interactions (Shweta et al., 2024). The therapeutic potential of 2-azetidinone derivatives, a class of heterocycles, has garnered considerable interest due to their diverse biological activities, including antibacterial, antifungal, anti-inflammatory, and anticonvulsant properties (Sulthana & Quine, 2015). Indeed, the structural versatility of the azetidinone ring allows for extensive chemical modifications, leading to a broad spectrum of pharmacological effects, including notable antibacterial efficacy against multi-drug resistant strains (Kusurkar et al., 2021). Molecular docking studies with 2-azetidinone derivatives have demonstrated strong binding affinities to various protein targets, including DNA gyrase, suggesting their utility as antibacterial agents (Sulthana & Quine, 2015). These in silico predictions highlight the potential of azetidinones as promising candidates for drug development, especially in combating resistant bacterial infections (Roman et al., 2023; Sulthana & Quine, 2015). Computational studies, such as molecular dynamics simulations, further investigate the stability and conformational flexibility of these ligand-protein complexes in physiologically relevant environments, providing a more comprehensive understanding of their inhibitory mechanisms (Muslim et al., 2023). Specifically, docking protocols often involve two primary steps: sampling ligand conformations within the active site of the protein and subsequently ranking these conformations using sophisticated scoring functions (Jain, 2024). These computational approaches are instrumental in early drug discovery projects, aiding in the design and development of novel molecules and enhancing project success rates while reducing development costs (Salih & Ali, 2023). This rigorous methodology ensures that only compounds with the most favorable binding characteristics are advanced to subsequent experimental stages, optimizing resource allocation. This integration of computational methodologies, ranging from molecular docking to dynamic simulations and comprehensive visualization, forms a robust framework for identifying and optimizing lead compounds, particularly novel 2-azetidinone derivatives, for targeted therapeutic interventions (Guguloth & Gubbiyappa, 2024).

## II. LITERATURE REVIEW

Recent advancements in computational chemistry have enabled more precise predictions of ligand-protein interactions, with particular emphasis on the structural elucidation of newly synthesized compounds like 2-azetidinones and their therapeutic implications (Bayrak et al., 2024). For instance, 2-azetidinone derivatives have shown significant antibacterial activity against various strains, including *Staphylococcus aureus*, *Bacillus subtilis*, *Escherichia coli*, and *Pseudomonas aeruginosa*, with some analogues exhibiting superior potency compared to standard drugs (Sulthana & Quine, 2015). Molecular docking studies have corroborated these findings, indicating strong binding affinities of these compounds to bacterial enzymes such as DNA gyrase, thereby elucidating their mechanism of action at a molecular level (Sulthana & Quine, 2015). These computational insights are further supported by studies demonstrating low free energy values for optimal binding interactions with various protein targets, including 1VQQ, 2WAE, 1PYY, and 1IYS, ranging from -6.5 to -7.9 kcal/mol, signifying stable and effective binding (Muslim et al., 2023). Furthermore, molecular dynamics simulations confirm the stability and tight binding of these lactozepine-derived compounds, showing consistent amino acid interactions within the protein-ligand complex (Muslim et al., 2024). Such comprehensive computational approaches not only identify potential drug candidates but also provide crucial information for optimizing their physicochemical properties to enhance target specificity and therapeutic efficacy (Muslim et al., 2024; Okella et al., 2022). This integrated computational approach, encompassing molecular docking and dynamic simulations, thus offers a powerful platform for rational drug design and optimization, particularly for novel scaffolds like 2-azetidinones (Mishra et al., 2024; Pei, 2024). This approach aids in the automated identification and preparation of target ligands, streamlining the virtual screening and lead optimization processes (Book, 2024). The utilization of in silico methods, including ligand preparation and protein receptor grid generation, alongside experimental techniques, substantially expedites the identification and optimization of promising drug candidates by providing detailed insights into their physicochemical

properties and biological activities (Çapan et al., 2024; Sulthana & Quine, 2015). This synergistic strategy allows for a more efficient selection of compounds for synthesis and biological evaluation, drastically reducing the overall drug discovery timeline. Such a streamlined process is critical for accelerating the translation of promising lead compounds from computational prediction to preclinical and clinical development stages. This refined drug discovery paradigm integrates both direct and indirect drug design techniques, significantly enhancing the identification of novel chemical entities with desirable therapeutic profiles (Mathpal et al., 2021). Moreover, advanced computational techniques, including molecular mechanics/generalized born surface area (MM/GBSA) and molecular mechanics/Poisson–Boltzmann surface area (MM/PBSA) calculations, are increasingly employed to evaluate binding free energies, offering a more nuanced understanding of protein-ligand complex stability and flexibility under physiological conditions (Rahman et al., 2025). These advanced computational methods, such as those employing AutoDock and Glide software, simulate binding interactions and predict the therapeutic potential of newly designed molecules like 2-azetidinones, thereby accelerating the discovery of lead compounds (Naithani & Guleria, 2024; Singh et al., 2025). This iterative process of computational design and experimental validation is crucial for developing novel therapeutic agents with improved efficacy and reduced side effects (Wu et al., 2023). Given that traditional drug discovery is a protracted and costly endeavor, computational tools have emerged as indispensable for modern pharmaceutical research, offering a more efficient and economical pathway to identify and optimize therapeutic agents (Naithani & Guleria, 2024; Wei & McCammon, 2024). These in silico methodologies are particularly valuable for exploring vast chemical spaces and prioritizing compounds for synthesis and biological evaluation, thus circumventing many of the limitations associated with traditional high-throughput screening (Padole et al., 2022; Sadybekov & Katritch, 2023).

## III. METHODOLOGY

This section outlines the specific computational and experimental protocols employed to investigate the binding characteristics and therapeutic potential of novel 2-azetidinone derivatives, focusing on their interactions with identified protein targets. This includes a detailed description of the molecular docking procedures, such as the selection of appropriate software and algorithms, as well as the parameters used for docking simulations to predict binding affinities and interaction modes. Subsequently, molecular dynamics simulations are conducted to assess the stability of the ligand-protein complexes over time and to observe the dynamic nature of their interactions within a simulated physiological environment (Alzain et al., 2025; Muslim et al., 2023). This comprehensive approach integrates in silico methodologies to elucidate the precise molecular mechanisms underpinning the therapeutic effects of these compounds, thereby facilitating the rational design of optimized drug candidates. The chosen methodology for molecular docking typically involves the use of established software like AutoDock Vina or Glide, often employing scoring functions such as XP to evaluate binding modes and affinities (Butini et al., 2024; Crisan, 2023). The generation of pdbqt files for docking simulations is frequently performed using tools like AutoDock Tools, which prepares both receptor and ligand files by assigning charges and adding hydrogens (Olazarán-Santibáñez et al., 2017). Moreover, the selection of appropriate protein targets, often retrieved from databases like the Protein Data Bank, is crucial for accurate predictions (Sulthana & Quine, 2015). Ligands, in turn, are meticulously prepared through modules like LigPrep, which generates multiple tautomers and stereoisomers to ensure comprehensive sampling of chemical space (Kumar et al., 2020). Preparation of the receptor protein is equally critical, involving optimization of hydrogen bond networks and refinement of the structure with restrained minimization to ensure accurate representation of the binding site (Chopra et al., 2018). For instance, one study specifically designed substituted amino benzoxazole-combined azetidinone ligands and evaluated them for breast cancer properties through molecular docking, ADME analysis, and pharmacophore modeling (Dheeraj et al., 2023). This rigorous computational approach, incorporating ADME and pharmacophore models, facilitates the prioritization of designed compounds by predicting critical physicochemical properties and biological activity spectra, thereby limiting the need

for extensive animal testing and reducing late-stage drug development failures (Begum et al., 2017; Hussein & Faisal, 2024). This strategic integration of in silico techniques significantly refines the drug discovery pipeline, ensuring that only the most promising compounds proceed to further validation stages. Subsequently, molecular dynamics simulations are performed using software packages such as GROMACS or AMBER, allowing for a detailed exploration of the ligand-receptor complex stability and conformational changes over a specified time duration under physiological conditions (Enni & Maraj, 2022). This analysis provides insights into critical interactions, including hydrogen bonds and hydrophobic contacts, which are essential for the observed binding affinity and specificity (Hussein & Faisal, 2024). Furthermore, ADMET predictions are performed using online resources such as admetSAR and Swiss ADME to assess the pharmacokinetics and potential toxicity of the compounds in the human body, thereby filtering out candidates with unfavourable properties early in the drug discovery process (Agu et al., 2023; Rasool et al., 2024). The initial step in molecular docking involves preparing the 3D structure of the target receptor, often obtained from experimental data, by adding missing atoms, assigning charges, and optimizing the protein structure (Shahab et al., 2024). Following this, a 3D grid is defined around the active site or binding pocket, delineating the spatial boundaries where ligands are expected to bind (Shahab et al., 2023). This grid ensures that the docking algorithm efficiently samples possible binding poses within a predefined region of interest (Kumar et al., 2022). The ligands, meticulously prepared with proper ionization states and minimized energy conformations using forcefields like OPLS-3E, are then flexibly docked into this defined grid, allowing for a comprehensive exploration of potential binding orientations and conformations ("Novel Thiazolidinedione Linked 1,3,4-Oxadiazole Derivatives as AXL Inhibitors Targeting Breast Cancer: In-Silico Design, ADMET Screening, and MM-GBSA Binding Free Energy," 2024).

The optimal poses are subsequently scored based on their binding affinity, often utilizing algorithms that account for van der Waals and electrostatic interactions, hydrogen bonding, and desolvation energies, thereby identifying the most energetically favorable ligand-receptor complexes (Yadav & Jaiswal, 2023).

- Ligand Preparation:

This subsection could detail the specific steps taken to prepare your 2-azetidinone derivatives, including energy minimization, tautomer generation, and 3D structure generation (e.g., using LigPrep or similar tools, and force fields like OPLS-3E) (Kumar et al., 2020; "Novel Thiazolidinedione Linked 1,3,4-Oxadiazole Derivatives as AXL Inhibitors Targeting Breast Cancer: In-Silico Design, ADMET Screening, and MM-GBSA Binding Free Energy," 2024).

- Protein Preparation and Grid Generation:

You could elaborate on how the target proteins were obtained (e.g., from the Protein Data Bank), cleaned, optimized (e.g., hydrogen bond networks, restrained minimization), and how the binding site grid was defined (Chopra et al., 2018; Shahab et al., 2023; Sulthana & Quine, 2015).

- Molecular Docking Parameters:

While mentioned, a dedicated subheading could clearly outline the specific software (e.g., AutoDock Vina, Glide), scoring functions (e.g., XP), and precision settings (e.g., "Extra Precision") used for your docking simulations (Butini et al., 2024; Crisan, 2023; Sulthana & Quine, 2015).

- Molecular Dynamics Simulation Setup:

If you perform MD simulations, a separate section detailing the simulation length, force field, water model, temperature, pressure coupling, and specific software (e.g., GROMACS, AMBER) would be valuable (Enni & Maraj, 2022).

- ADMET/Pharmacokinetic Predictions:

Although mentioned, a dedicated section in Methodology could specify the online resources (e.g., admetSAR, Swiss ADME) and models used for these predictions (Agu et al., 2023; Rasool et al., 2024).

- Visualization and Analysis Tools:

You could list and briefly describe the tools used for visualizing interactions (e.g., PyMol) and analyzing results (e.g., for pharmacophore models) (Dheeraj et al., 2023; PN et al., 2021). The specific parameters used for receptor grid generation, such as box size and grid spacing, are critical for accurately identifying potential binding sites and encompassing the entire protein molecule (Bhandare et al., 2022; Xiong et al., 2024). These grids are often generated using specialized modules that define the active site based on key residues or a user-defined geometric box,

ensuring comprehensive coverage of the putative binding region (Ramachandran et al., 2023). After defining the grid, the docking simulations are performed where the prepared ligands are allowed to explore various orientations and conformations within the binding pocket, typically employing search algorithms such as genetic algorithms or Monte Carlo simulations to identify optimal binding poses (Gadnayak et al., 2022). Subsequent to pose generation, consensus scoring, which integrates multiple algorithms, is frequently applied to mitigate individual model biases and enhance the reliability of predictive outcomes (Enni & Maraj, 2022).

## IV. RESULTS

The results section will present the outcomes of the computational studies, including detailed analyses of docking scores, binding poses, and interaction profiles for the synthesized 2-azetidinone derivatives with their respective target proteins. These results will be complemented by analyses of predicted pharmacokinetic properties, including ADME profiles, to assess the drug-likeness and bioavailability of the most promising compounds (Dheeraj et al., 2023; Kusurkar et al., 2021). The efficacy of these compounds as potential anti-cancer agents, for example, is further substantiated by their favorable docking scores with targets such as 4DBN, along with various hydrogen bond interactions, supporting their potential for good in vivo and in vitro activity (PN et al., 2021). Further in silico investigations, such as ADMET predictions, play a crucial role in assessing the pharmacokinetic and toxicological properties of these drug candidates, providing essential information for advancing them in the drug discovery pipeline (Faizan et al., 2024). This includes evaluating factors like oral bioavailability, metabolic stability, and potential toxicity, often through computational models that leverage established databases and algorithms (PN et al., 2021). Moreover, advanced tools like PyMol are frequently utilized to visualize and analyze these complex interactions in 3D, providing critical insights into hydrogen bonding, hydrophobic interactions, and pi-pi stacking that dictate binding affinity and specificity (PN et al., 2021). The generation of pharmacophore models also aids in identifying key structural features essential for biological activity and designing novel compounds with improved binding characteristics (Dheeraj et al., 2023). Ultimately, the integration of these computational strategies enables a more streamlined and cost-effective identification of potent and selective therapeutic agents, accelerating their translation from theoretical design to clinical application (Adebesin et al., 2022; Ali et al., 2025). This comprehensive approach, integrating advanced in silico analyses, significantly enhances the drug discovery pipeline by offering a robust framework for the rational design and optimization of novel therapeutic compounds (Hamed et al., 2025). Future work will involve synthesizing these promising derivatives and conducting in vitro and in vivo evaluations to validate their predicted therapeutic potential and explore broader spectrum activities, including against multidrug-resistant strains (Mehta et al., 2025; Verdino et al., 2017). This holistic strategy not only confirms their efficacy but also provides a deeper understanding of their mechanism of action, paving the way for targeted drug development (Ojuka et al., 2025). Such experimental validation is critical to translate computational predictions into tangible pharmaceutical interventions, particularly for challenging conditions where current therapies are insufficient (HR et al., 2025).

- Binding Affinity and Docking Score Analysis:

Detail the range of docking scores obtained for various compounds and target proteins, potentially including a table or chart summarizing key findings (Muslim et al., 2023).

- Detailed Interaction Profiles:

This section could focus on specific ligand-protein interactions, such as hydrogen bonding, hydrophobic interactions, pi-pi stacking, and the key amino acid residues involved, perhaps with specific examples and 3D visualization snapshots (Afolabi et al., 2024; Muhammad et al., 2019).

- Pharmacophore Model Development:

If you've developed pharmacophore models, a section explaining their features and implications for drug design would be appropriate (Dheeraj et al., 2023).

- ADMET/Pharmacokinetic Profiles of Promising Candidates:

Present the predicted ADME properties (e.g., oral bioavailability, metabolic stability, toxicity) for your most promising 2-azetidinone derivatives (Dheeraj et al., 2023; Kusurkar et al., 2021). These predictions offer critical insights into their potential oral bioavailability, metabolic stability, and overall drug-

likeness, guiding further experimental validation (Chakrabarti, 2023; Lukuzu et al., 2024). These computational analyses, including molecular docking and ADMET predictions, thus serve as a robust preliminary screening for identifying promising drug candidates, substantially accelerating the drug discovery process and reducing the reliance on costly and time-consuming experimental methods (Peng et al., 2024). This integrated in silico approach significantly enhances the identification of novel therapeutic agents, particularly for challenging conditions such as those involving antimicrobial resistance, by optimizing compound selection prior to resource-intensive wet-lab experimentation (Hassan et al., 2024; He, 2025). This allows for a more targeted synthesis of compounds, focusing on those with the highest predicted efficacy and safety profiles, thereby maximizing the chances of successful drug development (Lukuzu et al., 2024). Moreover, chemoinformatics tools expedite the screening of compound libraries, enabling rapid investigation of single compounds for multiple diseases and providing initial safety and toxicity profiles through ADMET testing, which traditionally is time and cost-intensive via in-vivo methods (Hassan et al., 2024). By predicting key characteristics such as mutagenicity, tumorigenicity, and reproductive effects, these in silico models allow researchers to identify and filter out potentially harmful compounds early in the drug discovery pipeline (Pattapulavar et al., 2025).

## V. DISCUSSION

The subsequent discussion will therefore focus on interpreting these computational findings within the broader context of anti-ulcer or other therapeutic potentials, highlighting correlations between structural features, predicted binding affinities, and ADMET profiles. This section will also address the limitations of the computational models and suggest further experimental validation strategies to confirm the in-silico predictions (Havryshchuk et al., 2025). For example, promising compounds identified through docking and ADMET analysis would ideally proceed to *in vitro* assays to validate their predicted inhibitory activity against the target enzymes and subsequently to *in vivo* studies to assess their therapeutic efficacy and safety (Guendouzi et al., 2024). Such subsequent investigations should encompass comprehensive *in vivo* pharmacokinetic profiling, toxicity assessments, and efficacy evaluations in relevant disease models to fully validate their safety and therapeutic potential (Hawash et al., 2025). Furthermore, the identification of specific amino acid residues involved in hydrogen bonding and hydrophobic interactions, such as those observed with VAL135, ILE322, and ASP128 for benzothiazole rings, offers critical insights into optimizing molecular structures for enhanced binding affinity and specificity (Afolabi et al., 2024; Muhammad et al., 2019). This detailed structural understanding will guide future rational drug design efforts, enabling the synthesis of compounds with improved pharmacological profiles and reduced off-target effects. Additionally, molecules demonstrating strong interactions with catalytic triad amino acids, even if they exhibit some off-targeting interactions, are often considered promising leads, although minimizing these off-target effects is crucial for enhanced specificity and reduced toxicity (Naithani et al., 2024). It is worth noting that compounds exhibiting potent activity as racemates, where both enantiomers contribute to inhibition, present a cost-effective option for development, especially when synthesized from achiral precursors (Sheikh et al., 2025). This can simplify the synthetic process and reduce manufacturing costs, making them attractive candidates for further development (Sheikh et al., 2025).

## VI. CONCLUSION

This detailed understanding of ligand-receptor interactions is crucial for the rational design of novel compounds with improved therapeutic profiles. This approach allows for a deeper exploration of the structure-activity relationships, enabling medicinal chemists to fine-tune molecular scaffolds for optimal therapeutic outcomes (Muhammad et al., 2019). The incorporation of aromatic ring characteristics in pharmacophore models, for instance, allows for the prioritization of compounds that can engage in advantageous π-π stacking interactions with specific amino acid residues in the binding pocket, thus enhancing binding stability and affinity (Asnawi et al., 2024). This iterative process of computational design, followed by *in vitro* and *in vivo* validation, ultimately accelerates the drug discovery pipeline by focusing experimental efforts on the most promising candidates (Faris et al., 2023). Moreover, such an integrated computational and experimental workflow is pivotal in identifying potential inhibitors, validating their mechanisms of action, and paving the way for the development of novel therapeutic agents (Divyashri et

al., 2020; Muhammad et al., 2019). Future research should also aim to integrate multi-omics data with these computational models to provide deeper insights into disease mechanisms and improve overall treatment outcomes (Sadia et al., 2024). It is imperative to conduct thorough experimental validation, including *in vitro* and *in vivo* studies, to confirm the computational predictions regarding efficacy and toxicity, as purely *in silico* findings require empirical corroboration (Babalola & Adegboyega, 2023; Liu et al., 2024). This comprehensive strategy, integrating advanced in silico analyses with rigorous experimental validation, significantly enhances the drug discovery pipeline by offering a robust framework for the rational design and optimization of novel therapeutic compounds (Ding et al., 2024). Structure-Activity Relationships: Given the mention of structural modifications and optimizing compounds, a dedicated discussion on SAR would strengthen your paper, linking specific structural features of 2-azetidinones to their predicted binding affinities and therapeutic potential (Muhammad et al., 2019). This would entail analyzing how variations in substituents on the azetidinone ring impact interactions with the target enzyme, thereby guiding the synthesis of more potent and selective inhibitors.

- Limitations of the Study:

While touched upon, a clear, separate heading for the limitations of your computational models and predictions would demonstrate a critical understanding of your work (Havryshchuk et al., 2025).

- Future Experimental Validation:

Expanding on the plan for *in vitro* and *in vivo* studies, perhaps with more specific aims or methods, could be a dedicated part of your conclusion or a separate "Future Work" section (Mehta et al., 2025; Verdino et al., 2017).

## REFERENCES


[1] Adebesin, A. O., Ayodele, A. O., Omotoso, O., Akinnusi, P. A., & Olubode, S. O. (2022). Computational evaluation of bioactive compounds from Vitis vinifera as a novel β-catenin inhibitor for cancer treatment. Bulletin of the National Research Centre/Bulletin of the National Research Center, 46(1). https://doi.org/10.1186/s42269-022-00872-3

[2] Afolabi, O. B., Olasehinde, O. R., Owolabi, O. V., Jaiyesimi, K. F., Adewumi, F. D., Idowu, O. T., Mabayoje, S. O., Obajuluwa, A. O., & Akpor, O. B. (2024). Insight into antioxidant-like activity and computational exploration of identified bioactive compounds in Talinum triangulare (Jacq.) aqueous extract as potential cholinesterase inhibitors. BMC Complementary Medicine and Therapies, 24(1). https://doi.org/10.1186/s12906-024-04424-2

[3] Agu, P. C., Afiukwa, C. A., Orji, O. U., Ezeh, E. M., Ofoke, I. H., Ogbu, C. O., Ugwuja, E. I., & Aja, P. M. (2023). Molecular docking as a tool for the discovery of molecular targets of nutraceuticals in diseases management [Review of Molecular docking as a tool for the discovery of molecular targets of nutraceuticals in diseases management]. Scientific Reports, 13(1). Nature Portfolio. https://doi.org/10.1038/s41598-023-40160-2

[4] Ali, I., Almostafa, M. M., Abbas, F., Younis, N. S., Khan, A. A., & Yahya, G. (2025). Computational discovery of BRD4 inhibitors for neuroblastoma therapy using pharmacophore screening and molecular simulations. Scientific Reports, 15(1). https://doi.org/10.1038/s41598-025-20714-2

[5] Alzain, A. A., Elbadwi, F. A., Osman, W., Ashour, A., Alqarni, M. H., Foudah, A. I., & Samra, R. M. (2025). Broadening the scope of bacteria DNA Gyrase B Inhibitors by marine compounds: Insights form molecular docking, MM-GBSA, molecular dynamics simulations and ADMET predictions. Scientific African, 28. https://doi.org/10.1016/j.sciaf.2025.e02658

[6] Asnawi, A., Mieldianisa, S., Aligita, W., Yuliantini, A., & Febrina, E. (2024). Integrative computational approaches for designing novel alpha-glucosidase inhibitors based on curculigoside A derivatives: Virtual screening, molecular docking, and molecular dynamics. Journal of Herbmed Pharmacology, 13(2), 308. https://doi.org/10.34172/jhp.2024.49407

[7] Azmatullah, S., Khan, A., Qazi, N. G., Nadeem, H., & Irshad, N. (2022). Pharmacological evaluation of newly synthesized organotin IV complex for antiulcer potential. BMC Pharmacology and Toxicology, 23(1). https://doi.org/10.1186/s40360-022-00596-0

[8] Babalola, B. A., & Adegboyega, A. E. (2023). Computational Discovery of Potent Imidazole Derivatives as Inhibitors of SARS-CoV-2 Main Protease: An Integrated Approach Combining Molecular Dynamics and Binding Affinity Analysis. Research Square (Research Square). https://doi.org/10.21203/rs.3.rs-3320696/v1

[9] Bayrak, H., Fahim, A. M., Boyracı, G. M., & Karahalil, F. Y. (2024). Synthesis, In Silico Studies, Antimicrobial, Antioxidant Activities, Docking Simulation, and Computational Analysis of Novel Acrylamide Derivatives. Russian Journal of General Chemistry, 94(8), 2044. https://doi.org/10.1134/s1070363224080188

[10] Begum, A., Begum, S., Prasad, K., & Bharathi, K. (2017). IN SILICO STUDIES ON FUNCTIONALIZED AZAGLYCINE DERIVATIVES CONTAINING 2, 4-THIAZOLIDINEDIONE SCAFFOLD ON MULTIPLE TARGETS. International Journal of Pharmacy and Pharmaceutical Sciences, 9(8), 209. https://doi.org/10.22159/ijpps.2017v9i8.19835

[11] Bhandare, R. R., Sigalapalli, D. K., Shaik, A. B., Canney, D. J., & Blass, B. E. (2022). Selectivity profile comparison for certain γ-butyrolactone and oxazolidinone-based ligands on a sigma 2 receptor over sigma 1: a molecular docking approach. RSC Advances, 12(31), 20096. https://doi.org/10.1039/d2ra03497b

[12] Book, A. (2024). Abstract Book. International Journal of Applied Pharmaceutics. https://doi.org/10.22159/ijap.2025v17i1.53183

[13] Butini, S., Grether, U., Jung, K., Ligresti, A., Allarà, M., Postmus, A. G. J., Maramai, S., Brogi, S., Papa, A., Carullo, G., Sykes, D. A., Veprintsev, D. B., Federico, S., Grillo, A., Guglielmo, B. D., Ramunno, A., Stevens, A. F., Heer, D., Lamponi, S., … Campiani, G. (2024). Development of Potent and Selective Monoacylglycerol Lipase Inhibitors. SARs, Structural Analysis, and Biological Characterization. Journal of Medicinal Chemistry, 67(3), 1758. https://doi.org/10.1021/acs.jmedchem.3c01278

[14] Çapan, İ., Hawash, M., Qaoud, M. T., Gülüm, L., Tunoğlu, E. N. Y., Çifci, K. U., Çevrimli, B. S., Sert, Y., Servi, S., Koca, İ., & Tutar, Y. (2024). Synthesis of novel carbazole hydrazine-carbothioamide scaffold as potent antioxidant, anticancer and antimicrobial agents. BMC Chemistry, 18(1). https://doi.org/10.1186/s13065-024-01207-1

[15] Chakrabarti, M. C. (2023). REVOLUTIONIZING ANTIMICROBIAL DRUG DISCOVERY: COMPUTATIONAL DESIGN AND ADMET STUDIES OF EMERGING POTENT ANTI-MICROBIAL AGENTS. International Journal of Pharmacy and Pharmaceutical Sciences, 28. https://doi.org/10.22159/ijpps.2023v15i8.48526

[16] Chopra, N., Kaur, K., & Kaur, S. (2018). Assessment of Antimicrobial, Anti-Inflammatory Activity and Docking Study of Novel 2-Arylimino-5-Indole-2-Yl-Methylidene-1, 3-Thiazolidine-4-one Derivatives. International Journal of Trend in Scientific Research and Development, 1097. https://doi.org/10.31142/ijtsrd18822

[17] Crisan, O. (2023). SYNTHESIS AND IN SILICO APPROACHES OF NEW SYMMETRIC BIS-THIAZOLIDINE-2,4-DIONES AS Ras AND Raf ONCOPROTEINS INHIBITORS. FARMACIA, 71(2), 254. https://doi.org/10.31925/farmacia.2023.2.4

[18] Dheeraj, G., Kumar, P., Apte, K., Ashtekar, H., & Dixit, S. R. (2023). Molecular docking, ADME analysis, and pharmacophore modelling of benzoxazole fused azetidinone derivatives as antibreast cancer agents. Annals of Phytomedicine an International Journal, 12(1). https://doi.org/10.54085/ap.2023.12.1.37

[19] Ding, H., Xing, F., Zou, L., & Zhao, L. (2024). QSAR analysis of VEGFR-2 inhibitors based on machine learning, Topomer CoMFA and molecule docking. BMC Chemistry, 18(1). https://doi.org/10.1186/s13065-024-01165-8

[20] Divyashri, G., Murthy, T. P. K., Sundareshan, S., Kamath, P., Murahari, M., Saraswathy, G. R., & Sadanandan, B. (2020). In silico approach towards the identification of potential inhibitors from Curcuma amada Roxb against H. pylori: ADMET screening and molecular docking studies. Bioimpacts, 11(2), 119. https://doi.org/10.34172/bi.2021.19

[21] El-Saghier, A. M. M., Enaili, S. S., Kadry, A. M., Abdou, A., & Gad, M. A. (2023). Green synthesis, biological and molecular docking of some novel sulfonamide thiadiazole derivatives as potential insecticidal against Spodoptera littoralis. Scientific Reports, 13(1). https://doi.org/10.1038/s41598-023-46602-1

[22] Enni, M. A., & Maraj, M. A. A. (2022). IN SILICO DRUG REPURPOSING FOR INFLAMMATORY DISEASES: A SYSTEMATIC REVIEW OF MOLECULAR DOCKING AND VIRTUAL SCREENING STUDIES [Review of IN SILICO DRUG REPURPOSING FOR INFLAMMATORY DISEASES: A SYSTEMATIC REVIEW OF MOLECULAR DOCKING AND VIRTUAL SCREENING STUDIES]. American Journal of Advanced Technology and Engineering Solutions, 2(4), 35. https://doi.org/10.63125/j1hbts51

[23] Faizan, S., Talath, S., Wali, A. F., Hani, U., Haider, N., Mandal, S. P., & Kumar, B. R. P. (2024). Anticancer potential of novel symmetrical and asymmetrical dihydropyridines against breast

cancer via EGFR inhibition: molecular design, synthesis, analysis and screening. RSC Advances, 14(16), 11368. https://doi.org/10.1039/d4ra01424c

[24] Faris, A., Edder, Y., Louchachha, I., Lahcen, I. A., Azzaoui, K., Hammouti, B., Merzouki, M., Challioui, A., Boualy, B., Karim, A., Hanbali, G., & Jodeh, S. (2023). From himachalenes to trans-himachalol: unveiling bioactivity through hemisynthesis and molecular docking analysis. Scientific Reports, 13(1). https://doi.org/10.1038/s41598-023-44652-z

[25] Gadnayak, A., Dehury, B., Nayak, A., Jena, S., Sahoo, A., Panda, P. C., Ray, A., & Nayak, S. (2022). 'Mechanistic insights into 5-lipoxygenase inhibition by active principles derived from essential oils of Curcuma species: Molecular docking, ADMET analysis and molecular dynamic simulation study. PLoS ONE, 17(7). https://doi.org/10.1371/journal.pone.0271956

[26] Guendouzi, A., Belkhırı, L., Djelti, F., Zendaoui, Z. M., Brahim, H., Guendouzi, A., Djekoun, A., & Boucekkine, A. (2024). In-silico design novel phenylsulfonyl furoxan and phenstatin derivatives as multi-target anti-cancer inhibitors based on 2D-QSAR, molecular docking, dynamics and ADMET approaches. Molecular Simulation, 50(6), 470. https://doi.org/10.1080/08927022.2024.2326180

[27] Guguloth, R., & Gubbiyappa, K. S. (2024). Synthesis, Docking and Biological Evaluation of New Series of Pyrrolidine Derivatives as Potent Antibacterial Agents. Asian Journal of Chemistry, 36(2), 489. https://doi.org/10.14233/ajchem.2024.31036

[28] Hamed, M. M., Ahmed, M., El-Dean, A. M. K., Alsedfy, M. Y., & Tolba, M. S. (2025). Thiopental-Inspired alkylpyrimidines as dual-target antimicrobial agents: Synthesis, biological activity, and molecular docking validation. Current Chemistry Letters, 14(4), 831. https://doi.org/10.5267/j.ccl.2025.8.001

[29] Hassan, S. S. ul, Wu, J., Li, T., Ye, X., Rehman, A., Yan, S., & Jin, H. (2024). Unlocking marine microbial treasures: new PBP2a-targeted antibiotics elicited by metals and enhanced by RSM-driven transcriptomics and chemoinformatics. Microbial Cell Factories, 23(1). https://doi.org/10.1186/s12934-024-02573-0

[30] Havryshchuk, L., Horishny, V. Ya., Ivasechko, I., Kozak, Y., Melnyk, D., Khyluk, D., Kusiy, M., Serhiyenko, V., Finiuk, N., Stoika, R., Holota, S., & Lesyk, R. (2025). Synthesis, anticancer properties evaluation and in silico studies of 2-chloro- and 2,2-dichloroacetamides bearing thiazole scaffolds. ScienceRise Pharmaceutical Science, 71. https://doi.org/10.15587/2519-4852.2025.323594

[31] Hawash, M., Ghannam, D., Dawoud, L., Dawoud, M. M. A., Ahmed, H. I., Alhajj, L., & Qaoud, M. T. (2025). Thiazole-carboxamide derivatives as potent antioxidant agents with drug-like properties: In vitro, molecular docking, and DFT studies. PLoS ONE, 20(9). https://doi.org/10.1371/journal.pone.0331000

[32] He, R. (2025). Enhancing Antimicrobial Molecule Prediction via Dynamic Routing Capsule Networks and Multi-Source Molecular Embeddings. arXiv (Cornell University). https://doi.org/10.48550/arxiv.2509.16571

[33] HR, A., Devi, K., BELIN, S., P, S. K. G., BAQI, M. A., VENKATHESHAN, N., Sucharitha, M. L., & JAYANTHI, K. (2025). EXPLORATION OF NICOTINOYL HYDRAZINE DERIVATIVES THROUGH IN SILICO STUDIES FOR NOVEL ANTI-TUBERCULAR DRUG DEVELOPMENT. International Journal of Applied Pharmaceutics, 534. https://doi.org/10.22159/ijap.2025v17i5.54697

[34] Hussein, A. A., & Faisal, M. (2024). In Silico Molecular Docking, Molecular Dynamics Simulation, and Pharmacokinetic prediction of Novel N-(2-(4-oxo-2-phenyl quinazoline-3(4H)-yl) Derivatives with Enhanced Anti-proliferative Activity. DergiPark (Istanbul University). https://dergipark.org.tr/en/pub/tcandtc/issue/90034/1556810

[35] Jain, S. (2024). Molecular Docking Analysis of D-Glucosamine and Rivastigmine Tartrate Targeting Alzheimer's Disease-Associated Proteins: An In Silico Approach. Asian Journal of Pharmaceutics, 18(2). https://doi.org/10.22377/ajp.v18i02.5458

[36] Kumar, A., Yadav, S., Singh, A. K., Kakkar, S., Narasimhan, B., & Sharma, A. (2022). Benzoxazole Derivatives: Qsar and Molecular Docking Studies. Research Square (Research Square). https://doi.org/10.21203/rs.3.rs-1780832/v1

[37] Kumar, S., Jang, C., Subedi, L., Kim, S. Y., & Kim, M. (2020). Repurposing of FDA approved ring systems through bi-directional target-ring system dual screening. Scientific Reports, 10(1). https://doi.org/10.1038/s41598-020-78077-9

[38] Kusurkar, R. V., Rayani, R. H., Vala, A., Parmar, D. R., Bhoi, M. N., Zunjar, V., & Soni, J. Y. (2021). Design, Synthesis, Molecular Docking and Biological Evaluation of Bromo-Pyridyl Containing 3-Chloro 2-Azetidinone Derivatives as Potential Antimycobacterial Agents. Research

Square (Research Square). https://doi.org/10.21203/rs.3.rs-699449/v1

[39] Liu, Y., Deng, L., Ding, F., Wang, Q., Zhang, S.-R., Mi, N., Zhang, W., Zeng, B., Tong, H., & Wu, L. (2024). Discovery of novel cholesteryl ester transfer protein (CETP) inhibitors by a multi-stage virtual screening. BMC Chemistry, 18(1). https://doi.org/10.1186/s13065-024-01192-5

[40] Lukuzu, T., Etey, N. B., Kavira, R., Nyampondo, N., Mulumba, B., Monsengo, J., Ebongya, N., Itoko, M., Nlandu, M., Matondo, A., Kafutshi, R. K., & Bambi-Nyanguile, S.-M. (2024). In vitro screening, molecular docking, and ADME Tox investigations for the design of novel beta-lactam antibiotics (Ampicillin and Ceftriaxone) derivatives as PBP2a inhibitors. Journal of Applied Biosciences, 197. https://doi.org/10.35759/jabs.197.6

[41] Mathpal, D., Masand, M., Thomas, A., Ahmad, I., Saeed, M., Zaman, G. S., Kamal, M., Jawaid, T., Sharma, P. K., Gupta, M. M., Kumar, S., Srivastava, S. P., & Balaramnavar, V. M. (2021). Pharmacophore modeling, docking and the integrated use of a ligand- and structure-based virtual screening approach for novel DNA gyrase inhibitors: synthetic and biological evaluation studies. RSC Advances, 11(55), 34462. https://doi.org/10.1039/d1ra05630a

[42] Mehta, S., Kaswan, P., Ranjan, P., & Sudesh. (2025). MOLECULAR DOCKING AND ADMET PROPERTIES OF NOVEL 5-METHYL-6AH-BENZO [4, 5] OXAZOLO [3,2-A] QUINOLIN-2-OL DERIVATIVES FOR THEIR ANTI-CANCER ACTIVITY. International Journal of Applied Pharmaceutics, 436. https://doi.org/10.22159/ijap.2025v17i5.54488

[43] Mishra, K. N., Rashmi, M., & Upadhyay, H. C. (2024). Coumarin-1,2,3-Triazole Hybrids as Promising Antibacterial Agents: In silico Molecular Docking, ADMET and Molecular Dynamics Simulation Studies (Exploring in silico Antibacterial Potential of Coumarin-1,2,3-triazoles). Indian Journal of Pharmaceutical Education and Research, 58(4), 1242. https://doi.org/10.5530/ijper.58.4.137

[44] Muhammad, M. B., Uzairu, A., Shallangwa, G. A., & Uba, S. (2019). MOLECULAR DOCKING AND QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIP (QSAR) STUDIES OF SOME SELECTED ANTI-ULCER INHIBITORS. The Journal of Engineering and Exact Sciences, 5(1), 100. https://doi.org/10.18540/jcecvl5iss1pp0100-0110

[45] Muslim, R. F., Guma, M. A., Abedulrahman, M. F., Ahmad, I., Patel, H., & Rabeea, M. A. (2023). Synthesizes, characterization, molecular modelling studies and bioactivity of a novel bicyclic compound of δ-lactam with oxazepine ring containing-sulphur substitute using an economic method. Research Square (Research Square). https://doi.org/10.21203/rs.3.rs-2972967/v1

[46] Muslim, R. F., Guma, M. A., Mahmood, A. A. R., Ahmad, I., Hirad, A. H., & Patel, H. (2024). Synthesizes, characterization, molecular modelling studies and bioactivity of a novel bicyclic compound of δ-lactam with oxazepine ring containing-sulphur substitute using an economic method. Journal of Computational Biophysics and Chemistry, 24(6), 733. https://doi.org/10.1142/s2737416524500807

[47] Naithani, K., Das, A., Ushare, M., Nath, S., Biswas, R., Kundu, A., Kazi, T. A., Mohan, U., & Bhowmik, S. (2024). Design, synthesis, and evaluation of 1,4-benzothiazine-3-one containing bisamide derivatives as dual inhibitors of Staphylococcus aureus with plausible application in a urinary catheter. Frontiers in Chemistry, 12. https://doi.org/10.3389/fchem.2024.1420593

[48] Naithani, U., & Guleria, V. (2024). Integrative computational approaches for discovery and evaluation of lead compound for drug design. Frontiers in Drug Discovery, 4. https://doi.org/10.3389/fddsv.2024.1362456

[49] Novel Thiazolidinedione Linked 1,3,4-Oxadiazole Derivatives as AXL Inhibitors Targeting Breast Cancer: In-Silico Design, ADMET Screening, and MM-GBSA Binding Free Energy. (2024). Jordan Journal of Biological Sciences, 17(1), 89. https://doi.org/10.54319/jjbs/170108

[50] Ojuka, P., Nyamato, G. S., Santos, C. B. R., & Kimani, N. M. (2025). A review and in silico screening of plant-derived snake venom/toxin inhibitors: ADMET, drug-likeness, and medicinal chemistry profiling [Review of A review and in silico screening of plant-derived snake venom/toxin inhibitors: ADMET, drug-likeness, and medicinal chemistry profiling]. PLoS Neglected Tropical Diseases, 19(10). Public Library of Science. https://doi.org/10.1371/journal.pntd.0013579

[51] Okella, H., Okello, E., Mtewa, A. G., Ikiriza, H., Kaggwa, B., Aber, J., Ndekezi, C., Nkamwesiga, J., Ajayi, C. O., Mugeni, I. M., Ssentamu, G., Ochwo, S., Odongo, S., Tolo, C. U., Kato, C. D., & Engeu, P. O. (2022). ADMET profiling and molecular docking of potential antimicrobial peptides previously isolated from African catfish, Clarias gariepinus. Frontiers in Molecular

Biosciences, 9. https://doi.org/10.3389/fmolb.2022.1039286

[52] Olazarán-Santibáñez, F. E., Bandyopadhyay, D., Carranza-Rosales, P., Rivera, G., & Balderas-Rentería, I. (2017). Stereochemical preference toward oncotarget: Design, synthesis and in vitro anticancer evaluation of diastereomeric β-lactams. Oncotarget, 8(23), 37773. https://doi.org/10.18632/oncotarget.18077

[53] Padole, S. S., Asnani, A. J., Chaple, D., & Katre, S. G. (2022). A review of approaches in computer-aided drug design in drug discovery [Review of A review of approaches in computer-aided drug design in drug discovery]. GSC Biological and Pharmaceutical Sciences, 19(2), 75. https://doi.org/10.30574/gscbps.2022.19.2.0161

[54] Pattapulavar, V., Ramanujam, S., Shah, M. R., Thirunavukkarasu, M. K., Arumugam, S., Ramanathan, K., Samrot, A. V., Deepasree, K., Venugopal, S., & Christopher, J. G. (2025). Streptomyces sp. VITGV156 secondary metabolite binds pathogenic protein PBP2a and Beta-lactamase. Frontiers in Bioinformatics, 5. https://doi.org/10.3389/fbinf.2025.1544800

[55] Pei, Z. (2024). Computer-aided drug discovery: From traditional simulation methods to language models and quantum computing. Cell Reports Physical Science, 102334. https://doi.org/10.1016/j.xcrp.2024.102334

[56] Peng, C., Zhang, X., Zhang, L., Yang, A., Wang, Y., & Chen, X. (2024). Integration of molecular docking and molecular dynamics simulations with subtractive proteomics approach to identify the novel drug targets and their inhibitors in Streptococcus gallolyticus. Scientific Reports, 14(1). https://doi.org/10.1038/s41598-024-64769-z

[57] PN, L., PT, M., & VIJAYAN, M. (2021). IN SILICO DESIGN OF BENOXAZOLE BEARING AZETIDINONE DERIVATIVES AS VEGFR-2 AGONIST IN CANCER. Asian Journal of Pharmaceutical and Clinical Research, 112. https://doi.org/10.22159/ajpcr.2021.v14i11.42706

[58] Rahman, M. O., Ahmed, S. S., Alqahtani, A. S., Rehman, M. T., Sultana, N., Bouhrim, M., Ali, M. A., & Lee, J. (2025). Identification of stigmasterol derived AChE inhibitors for Alzheimer's disease using high throughput virtual screening and molecular dynamics simulations. Scientific Reports, 15(1). https://doi.org/10.1038/s41598-025-20527-3

[59] Ramachandran, B., Saravanan, M., Jeyakanthan, J., & Lopes, B. S. (2023). Computational exploration of molecular flexibility and interaction of meropenem analogs with the active site of oxacillinase-23 in Acinetobacter baumannii. Frontiers in Chemistry, 11. https://doi.org/10.3389/fchem.2023.1090630

[60] Rasool, E. M. A., Anwaar, R., Naeem, A., Razzaq, A., Shoukat, S., Hameed, B., Abbas, M. N., & Shabbir, A. (2024). INTEGRATING BIOINFORMATICS TOOLS; MOLECULAR SCREENING FOR DRUG DISCOVERY AGAINST ESTROGEN POSITIVE BREAST CANCER. Journal of Population Therapeutics and Clinical Pharmacology. https://doi.org/10.53555/credtj09

[61] Roman, R., Pintilie, L., Nuță, D. C., Avram, S., Buiu, C., Sogor, C., & Limban, C. (2023). In Silico Prediction, Characterization and Molecular Docking Studies on New Benzamide Derivatives. Processes, 11(2), 479. https://doi.org/10.3390/pr11020479

[62] Sadia, H., Qureshi, I. Z., Naveed, M., Aziz, T., Alharbi, M., Alasmari, A. F., & Albekairi, T. H. (2024). Natural AI-based drug designing by modification of ascorbic acid and curcumin to combat buprofezin toxicity by using molecular dynamics study. Scientific Reports, 14(1). https://doi.org/10.1038/s41598-024-79275-5

[63] Sadybekov, A., & Katritch, V. (2023). Computational approaches streamlining drug discovery [Review of Computational approaches streamlining drug discovery]. Nature, 616(7958), 673. Nature Portfolio. https://doi.org/10.1038/s41586-023-05905-z

[64] Salih, T., & Ali, P. G. (2023). Rational design of novel compounds to serve as potential NDM-1 inhibitors using molecular docking, molecular dynamics simulation, and physicochemical studies. Research Square (Research Square). https://doi.org/10.21203/rs.3.rs-2488439/v1

[65] Shahab, M., Ziyu, P., Waqas, M., Zheng, G., Jardan, Y. A. B., Wondmie, G. F., & Bouhrhia, M. (2024). Targeting human progesterone receptor (PR), through pharmacophore-based screening and molecular simulation revealed potent inhibitors against breast cancer. Scientific Reports, 14(1). https://doi.org/10.1038/s41598-024-55321-0

[66] Shahab, M., Ziyu, P., Zheng, G., Almaary, K. S., Wondmie, G. F., & Bouhrhia, M. (2023). Targeting Human progesterone receptor (PR), through Pharmacophore- based screening and molecular simulation revealed potent inhibitors against breast cancer. Research Square (Research Square). https://doi.org/10.21203/rs.3.rs-3352678/v1

[67] Sheikh, H. K., Arshad, T., Khan, H., Habib, U., & Ortiz, C. J. C. (2025). Studies on racemic triglycerides as urease enzyme inhibitors. Bangladesh Journal of Pharmacology, 20(4), 140. https://doi.org/10.3329/bjp.v20i4.84324

[68] Shweta, S., Muhammad, S., Mishra, M. K., Chaudhry, A. R., & Ahmad, K. (2024). Synthesis, characterization, and biological activity using computational study of synthesized monocyclic β-lactam ligands. Research Square (Research Square). https://doi.org/10.21203/rs.3.rs-4365126/v1

[69] Singh, T., Shekhar, C., Singh, S., & Das, S. (2025). Integrating computational approaches to uncover β-lactamase-associated resistance in diarrheagenic Escherichia coli from pediatric patients. Scientific Reports, 15(1). https://doi.org/10.1038/s41598-025-16122-1

[70] Sulthana, R. M., & Quine, S. D. (2015). Synthesis, Characterization, Antibacterial Evaluation and Molecular Docking Studies of 2-Azetidinone Derivatives as Novel DNA Gyrase Inhibitors. International Letters of Chemistry Physics and Astronomy, 47, 94. https://doi.org/10.56431/p-l3nkhq

[71] Tripodi, F., Dapiaggi, F., Orsini, F., Pagliarin, R., Sello, G., & Coccetti, P. (2018). Synthesis and biological evaluation of new 3-amino-2-azetidinone derivatives as anti-colorectal cancer agents. MedChemComm, 9(5), 843. https://doi.org/10.1039/c8md00147b

[72] Verdino, A., Vigliottá, G., Giordano, D., Caputo, I., Soriente, A., Rosa, M. D., & Marabotti, A. (2017). Synthesis and biological evaluation of the progenitor of a new class of cephalosporin analogues, with a particular focus on structure-based computational analysis. PLoS ONE, 12(7). https://doi.org/10.1371/journal.pone.0181563

[73] Wei, H., & McCammon, J. A. (2024). Structure and dynamics in drug discovery. Npj Drug Discovery., 1(1). https://doi.org/10.1038/s44386-024-00001-2

[74] Wu, K., Karapetyan, E., Schloss, J. V., Vadgama, J. V., & Wu, Y. (2023). Advancements in small molecule drug design: A structural perspective [Review of Advancements in small molecule drug design: A structural perspective]. Drug Discovery Today, 28(10), 103730. Elsevier BV. https://doi.org/10.1016/j.drudis.2023.103730

[75] Xiong, F., Zhang, Y., Jiao, J., Zhu, Y., Mo, T., & Li, Y. (2024). Towards new bioactive fluorine-containing 1,3,4-oxadiazole-amide derivatives: synthesis, antibacterial activity, molecular docking and molecular dynamics simulation study. Molecular Diversity. https://doi.org/10.1007/s11030-024-10893-x

[76] Yadav, P., & Jaiswal, S. (2023). In-Silico Discovery of Potential Dual Inhibitors Targeting Human Acetylcholinesterase and Butyrylcholinesterase for Alzheimer's Disease: A Pharmacophore-Based Virtual Screening and Molecular Docking Approach. Research Square (Research Square). https://doi.org/10.21203/rs.3.rs-3757327/v1